

## Abstract

This invention provides an improved computationally derived regression-based method for determining IC<sub>50</sub> or EC<sub>50</sub> values for chemical compounds, which predicts potential drug-drug interactions involving cytochrome P450 and other enzymes, transporters, receptors or proteins with active site(s). In addition, this approach predicts affinity for target enzymes, transporters and receptor proteins from a single compound concentration, which will rapidly enable identification of therapeutic use.